

```
ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
31 32 33 34 35 36 37
ring/chain bonds:
7-11 8-12 9-10 12-13 13-14 13-15 13-16 14-17 15-24 16-31 17-18 18-19
19-20 20-21 21-22 22-23 24-25 25-26 26-27 27-28 28-29 29-30 31-32 32-33
33-34 34-35 35-36 36-37
ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds:
12-13 13-14 13-15 13-16 14-17 15-24 16-31 17-18 18-19 19-20 20-21 21-22
22-23 24-25 25-26 26-27 27-28 28-29 29-30 31-32 32-33 33-34 34-35 35-36
36-37
```

exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

## L1 STRUCTURE UPLOADED

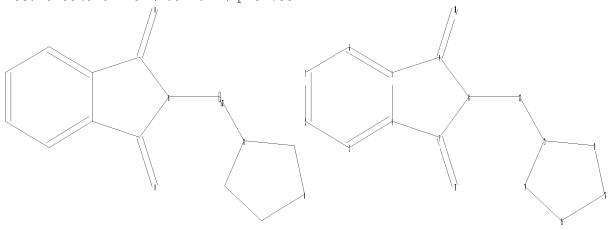
=> s l1 sss full FULL SEARCH INITIATED 11:19:43 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 772 TO ITERATE

100.0% PROCESSED 772 ITERATIONS 4 ANSWERS SEARCH TIME: 00.00.01

L2 4 SEA SSS FUL L1

=>

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ring nodes:
1 2 3 4 5 6 7 8 9 13 14 15 16 17

ring/chain nodes :

10 11 12

ring/chain bonds :

7-11 8-12 9-10 12-13

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-9 \quad 7-8 \quad 8-9 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17$ 

exact bonds :

4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17$ 

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

### L3 STRUCTURE UPLOADED

=> s 13 sss full

FULL SEARCH INITIATED 11:20:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3016 TO ITERATE

100.0% PROCESSED 3016 ITERATIONS

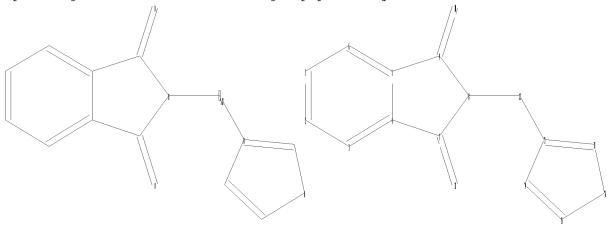
0 ANSWERS

SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L3

=>

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ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17

ring/chain nodes :

10 11 12

ring/chain bonds :

7-11 8-12 9-10 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

13-17 14-15

exact bonds :

4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

### L5 STRUCTURE UPLOADED

=> s 15 sss full

FULL SEARCH INITIATED 11:23:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5922 TO ITERATE

100.0% PROCESSED 5922 ITERATIONS

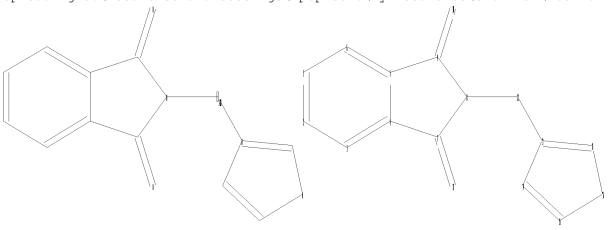
0 ANSWERS

SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L5

=>

 $\label{thm:locuments} \begin{tabular}{ll} Uploading C:\Documents and Settings\mpepitone\My Documents\ChemDraw\10572677\22.str$ 



ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17

ring/chain nodes :

10 11 12

ring/chain bonds :

7-11 8-12 9-10 12-13

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-9 \quad 7-8 \quad 8-9 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17$ 

exact/norm bonds :

13-17 14-15

exact bonds :

4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13

normalized bonds :

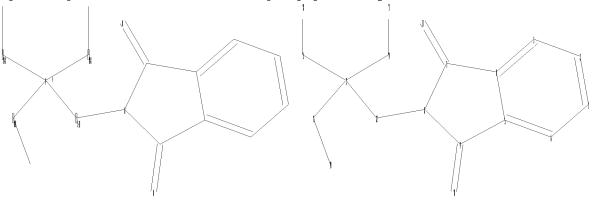
1-2 1-6 2-3 3-4 4-5 5-6 13-14 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

=>

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ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
10 11 12 13 14 15 16 17 18 19
ring/chain bonds:
7-11 8-12 9-10 12-13 13-14 13-15 13-16 14-17 15-18 16-19
ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds:
12-13 13-14 13-15 13-16 14-17 15-18 16-19
exact bonds:
4-7 5-9 7-8 7-11 8-9 8-12 9-10
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

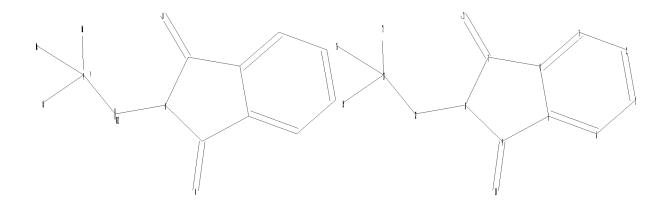
# Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS

#### L10 STRUCTURE UPLOADED

=> s 110 sss full STRUCTURE TOO LARGE - SEARCH ENDED A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>



chain nodes : 15 16 17 ring nodes : 1 2 3 4 5 6 7 8 9 ring/chain nodes : 10 11 12 13 chain bonds : 13-15 13-16 13-17 ring/chain bonds : 7-11 8-12 9-10 12-13 ring bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-9 \quad 7-8 \quad 8-9$ exact/norm bonds : 12-13 13-15 13-16 13-17 exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:CLASS

# L12 STRUCTURE UPLOADED

=> s 112 sss full FULL SEARCH INITIATED 11:35:05 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 2709 TO ITERATE

100.0% PROCESSED 2709 ITERATIONS 27 ANSWERS SEARCH TIME: 00.00.01

L13 27 SEA SSS FUL L12

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

189.24
986.54

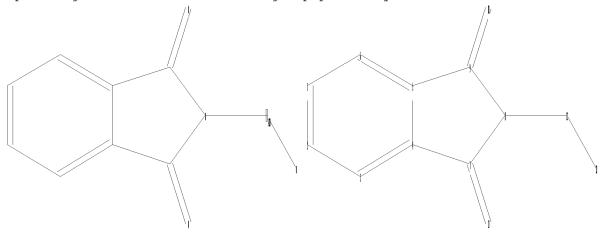
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

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chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

10 11 12

ring/chain bonds :

7-11 8-12 9-10 12-13

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-9 \quad 7-8 \quad 8-9$ 

exact bonds :

4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom

60140 ANSWERS

L15 STRUCTURE UPLOADED

=> s 115 sss full

FULL SEARCH INITIATED 11:39:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 268242 TO ITERATE

100.0% PROCESSED 268242 ITERATIONS

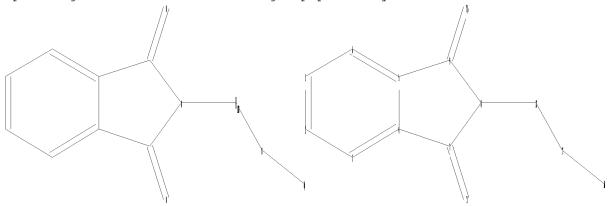
SEARCH TIME: 00.00.05

60140 SEA SSS FUL L15

=>

L16

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chain nodes : 13 16 ring nodes : 1 2 3 4 5 6 7 8 9 ring/chain nodes : 10 11 12 chain bonds : 13-16 ring/chain bonds : 7-11 8-12 9-10 12-13 ring bonds : 1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9exact/norm bonds : 13-16 exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 16:Atom

# L17 STRUCTURE UPLOADED

=> s 117 sss full FULL SEARCH INITIATED 11:41:44 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 266737 TO ITERATE

100.0% PROCESSED 266737 ITERATIONS 2397 ANSWERS SEARCH TIME: 00.00.08

L18 2397 SEA SSS FUL L17

=> file caplus

SINCE FILE 1011...
ENTRY SESSION
1436.06 COST IN U.S. DOLLARS FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

SINCE FILE TOTAL
ENTRY SESSION
0.00 -17.22

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STRUCTURE FILE UPDATES: 19 AUG 2009 HIGHEST RN 1174705-31-7 DICTIONARY FILE UPDATES: 19 AUG 2009 HIGHEST RN 1174705-31-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

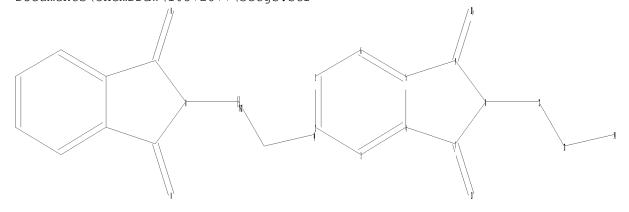
Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

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Documents\ChemDraw\10572677\setgs.str



chain nodes :
13 14
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
10 11 12
chain bonds :
12-13 13-14
ring/chain bonds :
7-11 8-12 9-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9

=> STR 671180-46-4

WARNING. SINGLE ATOM FRAGMENTS NOT INCLUDED IN MODEL:

Br

:END

L29 STRUCTURE CREATED

=> S L29 FAM FUL

FULL SEARCH INITIATED 11:52:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 27 TO ITERATE

100.0% PROCESSED 27 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

L30 2 SEA FAM FUL L29

=>

=> D SCAN

L30 2 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Isoindole-1,3(2H)-dione, 2-[10-(1H-imidazol-1-yl)decyl]-

MF C21 H27 N3 O2

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L30 2 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Isoindole-1,3(2H)-dione, 2-[10-(1H-imidazol-1-yl)decyl]-, hydrobromide (1:1)

MF C21 H27 N3 O2 . Br H